Parameterized Code Sharm-3D for Radiative Transfer Over Inhomogeneous Surfaces

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Abstract. This paper describes code SHARM-3D developed for fast and accurate simulations of the monochromatic radiance at the top of the atmosphere over spatially variable surfaces with Lambertian or anisotropic reflectance. The atmosphere is assumed to be laterally uniform across the image, and consisting of two layers with aerosols contained in the bottom layer. SHARM-3D performs simultaneous calculations for all specified incidence-view geometries and multiple wavelengths in one run. The numerical efficiency of the current version of code is close to its potential limit. This is achieved via two innovations. The first one is development of a comprehensive pre-computed look-up table of the 3D atmospheric optical transfer function for different atmospheric conditions. The second one is the use of a linear kernel model of the land surface bi-directional reflectance factor (BRF) in our algorithm that led to a fully parameterized solution in terms of the surface BRF parameters. The code is also able to model inland lakes and rivers. The water pixels are described with the Nakajima and Tanaka BRF model of wind-roughened water surface with the Lambertian offset. The latter is designed to approximately model reflectance of suspended matter or from the shallow bottom.

1. Introduction

The cloud-free atmospheric conditions play an important role in the spaceborne remote sensing of atmospheric aerosol and surface reflectance. Far from localized sources, aerosols vary on a much coarser scale than the surface reflectance. A recent analysis of mesoscale aerosol variability[1] gave the estimate of 20-60 km. Within such distances, the aerosol amount in atmospheric column and its radiative properties can often be considered approximately uniform, and all of the spatial and angular variability of the measured signal can be attributed to the variable surface reflectance. To model radiative transfer for this practically important case, we developed a Green's function (GF) method[2] that treats variability of the surface bi-directional reflectance factor (BRF), and includes 3D horizontal radiative transport caused by the surface inhomogeneity. The GF method rigorously decouples atmospheric transfer of radiation and the interactions of sunlight with the surface. It offers particular advantages when the atmosphere is laterally homogeneous, because solution for the atmospheric radiative transfer needs to be obtained only once for the whole area of interest. In the earlier work[3], we also parameterized the multiple reflections of photons from inhomogeneous surface. Implemented in code SHARM-3D, these features advanced the speed of calculations by a factor of ~10^3 as compared to code SHDOM[4], at the similar accuracy[3].

These improvements clarified further opportunities for the optimization. For example, the angular integration was originally performed for every surface pixel with its BRF in order to find the surface-reflected radiance, and to propagate it to the top of the atmosphere (TOA). Also, the 3D optical transfer function (OTF) had to be calculated each time the atmospheric conditions change, and these 3D computations were the lengthiest part of the total solution. These issues have been addressed in our recent research. As a result, we developed a comprehensive pre-calculated look-up table and a fast algorithm to reconstruct OTF for different atmospheric conditions. In addition, we implemented a

Li Sparse - Ross Thick[5] (LSRT) linear kernel model of the surface BRF in our algorithm that led to a fully parameterized solution in terms of the surface BRF parameters. This BRF model has been the basis of operational MODIS surface BRF/albedo algorithm[6], and it has shown very good performance globally in fitting the angular reflectance of natural land surfaces. Due to the linearity of this model, the requirement for the angular integration for every pixel is now reduced to only two integrations with predefined kernel functions, independently of the size of image. These two innovations raised the speed of calculations to its practical limit, and brought about by far the most efficient algorithm of the satellite image generation. The goal of this paper is to describe the new parameterizations, and to discuss performance of the latest version of code SHARM-3D, which can be downloaded from ftp://ltpftp.gsfc.nasa.gov/projects/asrvn/.

2. Parameterized SHARM-3D solution

2.1 Expression for the TOA Radiance

In the 3D Green's function solution[2], the top of the atmosphere (TOA) radiance at a given wavelength is expressed as a sum of path radiance (D) and surface-reflected radiance (L_s), directly and diffusely transmitted through the atmosphere. The diffusely transmitted signal is additionally split into the spatially averaged component and variation:

$$L(r-r_s;s_0,s)=D(s_0,s)\;+\;e^{-\tau/|\mu|}\,L_s(r;s_0,s)\;+\;\overline{L}_s^d(s_0,s)\;+\;\tilde{L}_s^d(r;s_0,s)\,. \quad (1)$$

Here, $r=(x,y)$ is a horizontal coordinate, r_s is a coordinate shift at the TOA for oblique view angles; τ is the optical thickness, and incidence (s_0) and view (s) directions are described by pairs of zenith and azimuthal angles (θ, φ). The surface-reflected radiance is expressed as:

$$L_s(r;s_0,s)\cong S_\lambda\mu_0 e^{-\tau/\mu_0}\,\{\,\rho(r;s_0,s)+\alpha c_0\rho_1(r;\mu)\overline{\rho}_2(\mu_0)\,\}\,+\,\frac{\alpha}{\pi}\int_{\Omega^+}D_s(s_0,s')\rho(r;s',s)\mu' ds'\,, \quad (2)$$

where πS_λ is extraterrestrial solar spectral irradiance, D_s is the surface-incident path radiance, ρ is the surface BRF, and

$$\rho_1(\mu)=\frac{1}{2\pi}\int_{\Omega^+}\rho(s',s)ds'\,,\;\;\rho_2(\mu_0)=\frac{1}{2\pi}\int_{\Omega^-}\rho(s_0,s)ds\,. \quad (3)$$

α is a multiple reflection factor, $\alpha=(1-\overline{q}(\mu_0)c_0)^{-1}$ depending on the mean surface albedo ($\overline{q}$) and spherical albedo of the atmosphere (c_0). The diffusely transmitted mean surface-reflected radiance at the TOA is calculated from L_s with the help of 1D diffuse Green's function of the atmosphere[7]:

$$\overline{L}_s^d(s_0,s)\;=\;\int_{\Omega^-}G^d(s_1,s)\overline{L}_s(s_0,s_1)ds_1\,. \quad (4)$$

In the literature, function πG^d is often called bi-directional upward diffuse transmittance of the atmosphere. The surface albedo is defined as a ratio of reflected and incident surface fluxes:

$$q(r;\mu_0)=F^{Up}(r;\mu_0)\,/\,\overline{F}^{Down}(\mu_0)\,, \quad (5a)$$

$$\overline{F}^{Down}(\mu_0)=\pi S_\lambda\mu_0 e^{-\tau/\mu_0}+\int_{\Omega^+}D_s(s_0,s')\mu' ds'=F_s^{Dir}(\mu_0)+F_s^{Dif}(\mu_0)\,, \quad (5b)$$

$$F^{Up}(r;\mu_0)=\pi S_\lambda\mu_0 e^{-\tau/\mu_0}q_2(r;\mu_0)+\int_{\Omega^+}\mu' q_2(r;\mu')D_s(s_0,s')ds'\,,\;\;q_2(r;\mu')=\frac{1}{\pi}\int_{\Omega^-}\rho(r;s_0,s)\mu ds\,. \quad (5c)$$

Finally, the diffusely transmitted variation of surface-reflected radiance is given by:

$$\tilde{L}_s^d(r - r_s; \mu_0; s) \cong \frac{\alpha E_0(\mu_0)}{(2\pi)^2} \int_{-\infty}^{+\infty} \frac{\tilde{q}(\mu_0; p) A(p; s)}{1 - \bar{q}(\mu_0) c(p)} e^{-i[p(r - r_s) - \Phi(p;s)]} dp \,. \tag{6}$$

Here, $\pi E_0(\mu_0) = \bar{F}^{Down}(\mu_0)$ is surface irradiance, $\tilde{q}(p)$ is a Fourier-transform of albedo variation at spatial frequency $p=(p_x,p_y)$, A and Φ are the amplitude and phase of the atmospheric optical transfer function (OTF_L), and $c(p)$ is spherical albedo of atmosphere at spatial frequency p. The details of derivation and notations are fully explained elsewhere[2,7].

The described formulas employ several parameterizations. For example, the multiple reflections between the atmosphere and anisotropically reflecting surface are parameterized in Eq. (2). Eq. (6) uses a Lambertian approximation, and neglects the non-linear interactions of variation of surface reflectance. These parameterizations immensely simplify the radiative transfer algorithm and gain a speed advantage of up to a factor of 10^3 as compared to SHDOM, yet retain the high accuracy,[4] which is generally better than 1%.

2. Parameterized Solution with LSRT BRF Model

In 1992, Roujean et al.[8] introduced a concept of linear kernel-based BRF model. One model of this family is a semi-empirical LSRT model[5] represented as a sum of Lambertian, geometric-optical, and volume scattering components:

$$\rho(s', s) = k_L + k_{go} f_{go}(s', s) + k_v f_v(s', s) \,. \tag{7}$$

It uses predefined "kernels" f_{go}, f_v to describe different angular shapes. The kernels are independent of the land conditions. The BRF of a pixel is characterized by a combination of three kernel weights, $\vec{K} = \{k_L, k_{go}, k_v\}^T$. The processing of MODIS[6] and MISR[9] global satellite data shows that LSRT model fits well the diversity of natural BRF shapes. This model is widely used in the applied research.

Use of LSRT model offers an immediate advantage of parameterizing our analytical solution into a weakly non-linear function of spatially variable kernel weights with angular-dependent coefficients that need to be calculated only once for the whole image. Because the following formulation uses azimuthal harmonics, let us first define an azimuthal Fourier expansion:

$$h(\varphi - \varphi') = \sum_{m \ge 0}^{\infty} (2 - \delta_{0,m}) h^{(m)} \cos m(\varphi' - \varphi) \,, \; h^{(m)} = \frac{1}{2\pi} \int_0^{2\pi} h(\varphi') \cos m\varphi' d\varphi' \,. \tag{8}$$

Below, the subscript k will refer to either geometric-optical (go) or volumetric (v) kernels. Let us now introduce a set of the required integral functions:

$$f_k^1(\mu) = \frac{1}{2\pi} \int_0^1 d\mu' \int_0^{2\pi} f_k(\mu', \mu, \varphi' - \varphi) d\varphi' = \int_0^1 f_k^{(0)}(\mu', \mu) d\mu' \,, \tag{9a}$$

$$f_k^2(\mu_0) = \frac{1}{2\pi} \int_{-1}^0 d\mu_1 \int_0^{2\pi} f_k(\mu_0, \mu_1, \varphi - \varphi_0) d\varphi = \int_{-1}^0 f_k^{(0)}(\mu_0, \mu_1) d\mu_1 \,, \tag{9b}$$

$$f_k^3(\mu') = \frac{1}{\pi} \int_{-1}^0 \mu d\mu \int_0^{2\pi} f_k(\mu', \mu, \varphi - \varphi') d\varphi = 2 \int_{-1}^0 f_k^{(0)}(\mu', \mu) \mu d\mu \,. \tag{9c}$$

Based on these definitions, the functions ρ_1, ρ_2 (Eq. (3)) become:

$$\rho_1(r;\mu) = k_L(r) + k_{go}(r)\, f_{go}^{1}(\mu) + k_v(r)\, f_v^{1}(\mu)\,, \tag{10a}$$

$$\bar{\rho}_2(\mu_0) = \bar{k}_L + \bar{k}_{go}\, f_{go}^{2}(\mu_0) + \bar{k}_v\, f_v^{2}(\mu_0)\,. \tag{10b}$$

The surface albedo splits into the direct and diffuse components according to the source of irradiance:

$$q(r;\mu_0) = q^{Dir}(r;\mu_0) + q^{Dif}(r;\mu_0)\,, \tag{10c}$$

$$q^{Dir}(r;\mu_0) = \frac{F_s^{Dir}(\mu_0)}{\pi E_0(\mu_0)}\{k_L(r) + k_{go}(r)\, f_{go}^{3}(\mu_0) + k_v(r)\, f_v^{3}(\mu_0)\}\,, \tag{10d}$$

$$q^{Dif}(r;\mu_0) = E_0^{-1}(\mu_0)\{k_L(r)\frac{F_s^{Dif}(\mu_0)}{\pi} + k_{go}(r) D_{go}^{3}(\mu_0) + k_v(r) D_v^{3}(\mu_0)\}\,, \tag{10e}$$

where

$$D_k^3(\mu_0) = 2\int_0^1 \mu' f_k^{3}(\mu') D_s^{(0)}(\mu_0,\mu') d\mu'\,. \tag{10f}$$

The surface-reflected radiance $L_s(r;s_0,s)$ is expressed via functions:

$$D_k^1(s_0,s) = \frac{1}{\pi}\int_0^1 \mu' d\mu' \int_0^{2\pi} d\varphi' D_s(\mu_0,\mu',\varphi'-\varphi_0)\, f_k(\mu',\mu,\varphi-\varphi') =$$

$$= \sum_{m\ge 0}^{\infty}(2-\delta_{0,m}) D_k^{1(m)}(\mu_0,\mu)\cos m(\varphi-\varphi_0)\,, \tag{11a}$$

$$D_k^{1(m)}(\mu_0,\mu) = 2\int_0^1 D^{(m)}(\mu_0,\mu')\, f_k^{(m)}(\mu',\mu)\mu' d\mu'\,. \tag{11b}$$

The mean diffusely transmitted radiance $\bar{L}_s^d(s_0,s)$ depends on the following functions:

$$G^{av}(\mu) = \int_{-1}^{0} d\mu_1 \int_0^{2\pi} G^d(\mu_1,\mu,\varphi-\varphi_1) d\varphi_1 = 2\pi \int_{-1}^{0} G^{d(0)}(\mu_1,\mu) d\mu_1\,; \tag{11c}$$

$$G_k^{11}(\mu) = \int_{-1}^{0} f_k^1(\mu_1) d\mu_1 \int_0^{2\pi} G^d(\mu_1,\mu,\varphi-\varphi_1) d\varphi_1 = 2\pi \int_{-1}^{0} f_k^1(\mu_1) G^{d(0)}(\mu_1,\mu) d\mu_1\,; \tag{11d}$$

$$G_k^1(s_0,s) = \int_{-1}^{0} d\mu_1 \int_0^{2\pi} G^d(\mu_1,\mu,\varphi-\varphi_1)\, f_k(\mu_0,\mu_1,\varphi_1-\varphi_0) d\varphi_1 =$$

$$\sum_{m\ge 0}^{\infty}(2-\delta_{0,m}) G_k^{1(m)}(\mu_0,\mu)\cos m(\varphi-\varphi_0)\,, \tag{11e}$$

$$G_k^{1(m)}(\mu_0,\mu) = 2\pi\int_0^1 G^{(m)}(\mu_1,\mu)\, f_k^{(m)}(\mu_0,\mu_1) d\mu_1\,; \tag{11f}$$

$$H_k^1(s_0,s) = \int_{-1}^{0} d\mu_1 \int_0^{2\pi} G^d(\mu_1,\mu,\varphi-\varphi_1) D_k^1(\mu_0,\mu_1,\varphi_1-\varphi_0) d\varphi_1 =$$

$$\sum_{m\ge 0}^{\infty}(2-\delta_{0,m}) H_k^{1(m)}(\mu_0,\mu)\cos m(\varphi-\varphi_0)\,, \tag{11g}$$

$$H_k^{1(m)}(\mu_0,\mu) = 2\pi\int_0^1 G^{(m)}(\mu_1,\mu)D_k^{1(m)}(\mu_0,\mu_1)d\mu_1\,. \tag{11h}$$

With the introduced functions, the surface-reflected radiance at the bottom of atmosphere and the mean surface signal diffusely transmitted at TOA in Eq. (1) can be written as follows:

$$\begin{aligned} L_s(r;s_0,s) \cong\ & \mathrm{S}_\lambda \mu_0 e^{-\tau(\frac{1}{\mu_0}+\frac{1}{|\mu|})}\{\,\rho(r;s_0,s)+\alpha c_0\rho_1(r;\mu)\ \overline{\rho}_2(\mu_0)\,\}\ + \\ & e^{-\tau/|\mu|}\,\alpha[k_L(r)E_0^d(\mu_0)+k_{go}(r)D_{go}^1(s_0,s)+k_v(r)D_v^1(s_0,s)]\,; \end{aligned} \tag{12a}$$

$$\begin{aligned} \overline{L}_s^d(s_0,s) =\ & \mathrm{S}_\lambda \mu_0 e^{-\tau/\mu_0}\{[\overline{k}_L G^{av}(\mu)+\overline{k}_{go}G_{go}^1(s_0,s)+\overline{k}_v G_v^1(s_0,s)]+ \\ & \alpha c_0\,[\overline{k}_L G^{av}(\mu)+\overline{k}_{go}G_{go}^{11}(\mu)+\overline{k}_v G_v^{11}(\mu)]\ \overline{\rho}_2(\mu_0)\,\}\ + \\ & \alpha[\overline{k}_L E_0^d(\mu_0)G^{av}(\mu)+\overline{k}_{go}H_{go}^1(s_0,s)+\overline{k}_v H_v^1(s_0,s)]\,. \end{aligned} \tag{12b}$$

The described algorithm (Eqs. 1, 12) uses two different solutions of code SHARM. The first one is a standard solution with the atmosphere illuminated at the top. It provides the path radiance at TOA along with its azimuthal harmonics at the bottom of the atmosphere, surface irradiance, atmospheric transmittance and spherical albedo. In the second solution, the atmosphere is illuminated from the bottom; in other words, it corresponds to a reversed order of atmospheric layers[7]. This solution provides azimuthal harmonics of the Green's function in the multiple scattering. Because aerosol scattering may cause the Green's function to be very asymmetric in the aureole region, the harmonics of the single-scattering term are calculated separately using the high-order gaussian quadrature for azimuthal angle (N_{SS}=129). With this separation, a relatively low order of MSH (*nb*=24-36) can be used in the multiple scattering calculations. This approach reduces the overall computing time and preserves the total accuracy. Eqs. (11-a, -e, -g) show that the integration in azimuth is performed very efficiently by summation of the azimuthal Fourier series. The zenith angle integration uses Gaussian quadrature of the order N_q=*nb*/2+10. Because Legendre polynomial of the order 2*N* is integrated exactly with the quadrature of the order *N*, and the kernels f_{go}, f_v can be approximated by the low order polynomials, the quadrature N_q warrants accurate integration.

3. Parameterization of Atmospheric OTF

Until recently, computing OTF for given atmospheric conditions consumed most of the time required by SHARM-3D algorithm. In this work, we develop a look-up table (LUT) algorithm that allows to compactly store certain pre-calculated functions, and to reconstruct the full OTF from the LUT based on the symmetry and scaling properties of OTF. To build an efficient algorithm, we divide the atmosphere into two vertical layers with Rayleigh scattering and gaseous absorption. The aerosols confined to the bottom layer.

Let us give a definition of the atmospheric optical transfer function, and derive a formula in the first order of scattering in order to establish the required properties of OTF. Below, *z*-axis starts at TOA and aims towards the surface (SHARM convention).

3.1. Single Scattering OTF

OTF is a spatial Fourier-transform of the atmospheric point-spread function (PSF), and is found from the following boundary-value problem[10,11,2]:

$$\mu \frac{\partial \Psi(z;p;s_0,s)}{\partial z} + [\alpha(z) - i(p,\nu)]\Psi(z;p;s_0,s) = \frac{\sigma(z)}{4\pi}\int_{\Omega} \chi(z;s',s)\Psi(z;p;s_0,s')ds' , \tag{13a}$$

$$\Psi(0;p;s_0,s) = 0,\ \mu>0;\ \Psi(H;p;s_0,s) = \delta(s-s_0),\ \mu<0. \tag{13b}$$

Above, α and σ are extinction and scattering coefficients, $\boldsymbol{p}$ is a vector of spatial frequency $p = (p_x, p_y)$, and ν is a projection of vector of direction on the horizontal plane $\nu = (\sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi)$. In Eq. (13b), s_0 is the direction of source beam illuminating the atmosphere from below, and s is view direction. Because OTF is a complex function, it can be represented via its amplitude and phase:

$$\Psi(z;p;s_0,s) = e^{\frac{i(p,\nu)(H-z)}{|\mu|}}\{e^{-\frac{\tau_0-\tau(z)}{|\mu|}}\delta(s-s_0) + A(z;p;s_0,s)e^{i\Phi(z;p;s_0,s)}\}. \tag{14}$$

The first term on the right-hand side of equation (14) explicitly takes into account the phase shift at oblique view angles. Let us derive an expression for the single-scattering component of the diffuse OTF using the method of successive orders of scattering. Following a similar study[12], we represent OTF as a sum of direct, single scattered and multiple scattered components:

$$\Psi = \Psi^{(0)} + \Psi^{(1)} + \Psi^{(m)}. \tag{15}$$

The direct component obeys the problem:

$$\mu \frac{\partial \Psi^{(0)}(z)}{\partial z} + [\alpha(z) - i(p,\nu)]\Psi^{(0)}(z) = 0; \tag{16a}$$

$$\Psi^{(0)}(0) = 0,\ \mu>0;\ \Psi^{(0)}(H) = \delta(s-s_0),\ \mu<0, \tag{16b}$$

and has the following solution:

$$\Psi^{(0)}(z;p;s_0,s) = \begin{cases} \exp\{-\frac{\tau_0 - \tau(z) - i(p,\nu)(H-z)}{|\mu|}\}\delta(s-s_0), \mu<0 \\ 0, \quad \mu>0 \end{cases}. \tag{17}$$

Now one can formulate the problem for the single scattering OTF:

$$\mu \frac{\partial \Psi^{(1)}(z)}{\partial z} + [\alpha(z) - i(p,\nu)]\Psi^{(1)}(z) = \frac{\sigma(z)}{4\pi}\exp\{-\frac{\tau_0 - \tau(z) - i(p,\nu_0)(H-z)}{|\mu_0|}\}\ \chi(z;s_0,s); \tag{18a}$$

$$\Psi^{(1)}(0) = 0,\ \mu>0;\ \Psi^{(1)}(H) = 0,\ \mu<0. \tag{18b}$$

Let us denote $\varepsilon = \frac{(p,\nu)}{|\mu|} = |tg\theta|\{p_x\cos\varphi + p_y\sin\varphi\}$, and consider a homogeneous atmosphere for simplicity. Then the diffuse OTF in the upward direction at TOA, after subtraction of the phase shift, is given by:

$$Z = Ae^{i\Phi} = \frac{\tau_0\omega\chi(s_0,s)}{4\pi|\mu|}\{e^{-\frac{\tau_0}{|\mu|}} - e^{-\frac{\tau_0}{|\mu_0|}+i(\varepsilon_0-\varepsilon)H}\}/[\tau_0(|\mu_0|^{-1} - |\mu|^{-1}) + i(\varepsilon-\varepsilon_0)H]. \tag{19a}$$

In the singularity point $s = s_0$,

$$A(s=s_0) = \frac{\tau_0\omega\chi(0)}{4\pi|\mu_0|}e^{-\frac{\tau_0}{|\mu_0|}},\ \Phi(s=s_0) = 0. \tag{19b}$$

Later we will also need a solution for the two-layer atmosphere, which in the single scattering is a sum of contributions from the bottom layer ($z_1 \le z \le H$), and the top layer ($0 \le z < z_1$):

$$Z(0;H) = e^{-\frac{\tau(z_1)}{|\mu|}} Z(z_1;H) + Z(0;z_1)\,. \qquad (20)$$

Solution given by Eq. (19a) corresponds to the mono-directional (beam) source of light. The function OTF_L required by Eq. (6) corresponds to isotropic (Lambert) illumination, and it is obtained by an additional integration over the directions of origin:

$$\Psi_L^{(1)}(s) = \int_{\Omega^-} \Psi^{(1)}(s_0, s) ds_0\,. \qquad (21)$$

3.2 Development of LUT and properties of OTF

To compute the function OTF_L we developed a rigorous algorithm of method of spherical harmonics[13] (MSH). It solves problem (13) with the low boundary condition $\Psi(H;s) = 1$ (μ<0), which follows from Eq. (21). The MSH algorithm works reliably for low and medium spatial frequencies, p≤2-10, depending on aerosol stratification in the atmosphere. At higher p, oscillations of the complex term degrade convergence of the algorithm. On the other hand, the fraction of the multiple scattering in the solution quickly decreases with increase of p. For this reason, at $p>p_{ss}=2$ we calculate OTF in the single scattering with numeric integration of Eq. (21) using the high-order Gaussian quadrature to ensure stable results. Analysis of the full solution (Eq. 1) for variety of scenes shows that the error due to this approximation is negligible. These results agree with the study[12].

The look-up table of OTF_L should be representative of different atmospheric conditions, and should factor in the following dimensions:
1) wavelength, 2) aerosol model, 3) vertical profile of aerosol, 4) aerosol optical thickness, 5) spatial frequency and view angles (p_x, p_y ; μ, φ). To eliminate dependence on wavelength, we split the total problem into two sub-problems: *i*) development of the separate look-up tables for the aerosol and molecular atmospheres, and *ii*) calculation of atmospheric OTF_L for the aerosol-molecular mixture.

First, let us consider the properties of OTF_L useful for developing the aerosol LUT.

a) Dependence on phase function

Due to integration (Eq. (21)), the diffuse OTF_L depends on some integral parameter of phase function related to its asymmetry rather than on its specific shape. Below, we will characterize the asymmetry with the first Legendre expansion coefficient (x_1).

b) Dependence on single scattering albedo

As Eq. (19a) shows, the amplitude $A^{(1)}$ is proportional to the single scattering albedo, $A^{(1)} \propto \omega$. Generally, $A^{(n)} \propto \omega^n$, while phase does not depend on ω. Also, at p=0 the OTF_L coincides with the 1D atmospheric transmission in the upward direction $T(\omega;\mu) = e^{-\tau_0/|\mu|} + T^d(\omega;\mu)$, in other words $A(p=0;\omega,\mu) = T^d(\omega,\mu)$. The transmission function is routinely computed by code SHARM when calculating the path radiance (see sec. 2). This consideration shows that it is sufficient to build aerosol LUT for some reference single scattering albedo, ω_0. Then the amplitude can be accurately found for the single scattering range as:

$$A(p;\omega) = \beta(p_{ss}) A(p;\omega_0)\,,\ \beta(p_{ss}) = \frac{\omega}{\omega_0}\,,\ p \ge p_{ss}. \qquad (22a)$$

At p=0, the scaling is also exact with $\beta(0) = \dfrac{T^d(\omega;\mu)}{A(p=0;\omega_0;\mu)}$. Assuming that the scaling coefficient decreases linearly with spatial frequency, we get the following approximation in parameter ω for the intermediate multiple-scattering range:

$$A(p;\omega) = \{\beta(0) - \frac{\beta(0)-\beta(p_{ss})}{p_{ss}} p\} A(p;\omega_0)\,,\ \ 0 \le p < p_{ss}. \tag{22b}$$

The described interpolation algorithm eliminates the ω-dimension of the aerosol LUT.

c) Scaling property of OTF

A scaling property of OTF eliminates dependence on the aerosol vertical profile. The single scattering solution (19a) shows that OTF depends on the product of frequency and height of scattering layer pH rather than on parameters p and H separately. This property can be established by analysis of Eq. (13) in successive orders of scattering, and can be verified with the multiple scattering MSH solution. Thus, the LUT needs to be calculated only for some standard aerosol profile with an equivalent height of layer H_0^{eq} (defined for the multi-layer atmosphere as $H^{eq} = \sum H_i\sigma_i / \sum \sigma_i$). Then, for the profile with an equivalent height H^{eq}, the OTF can be found by scaling the frequency p with the factor of H_0^{eq} / H^{eq}.

d) Symmetry properties of OTF

Given atmospheric conditions, the diffuse OTF_L at TOA is a function of four parameters (p_x, p_y , μ, φ). The x-, and y- projections of spatial frequency are free parameters of problem (13) varying independently in the range [- $p_{Nyquist}$, + $p_{Nyquist}$], which can be very large. This fact alone could make the LUT approach unfeasible because of the sheer size of the look-up table. However, the symmetry properties of OTF_L eliminate one of p-dimensions and permit to store OTF in a very compact form.

Because the light source at the surface is isotropic, both PSF_L and OTF_L have a cylindrical symmetry[11] and are rotationally invariant. This suggests that OTF_L has a dimension of three rather than four, and

$$\Psi_L(\mu; p_x, p_y, \varphi) = \Psi_L(\mu; p_1, 0; \varphi_1)\,, \tag{23a}$$

where the new coordinates are related by rotational transformation:

$$p_1 = \sqrt{p_x^2 + p_y^2}\,,\ \varphi_1 = \varphi - arctg(\frac{p_y}{p_x})\,. \tag{23b}$$

So, given the view zenith angle, function $\Psi_L(\mu; p_x, p_y, \varphi)$ can be reconstructed from $\Psi_L(\mu; p_1; \varphi_1)$ if it were calculated for different spatial frequencies and all possible azimuths (p_1, φ_1) defined by condition (23b).

Yet another symmetry property of the function $\Psi_L(\mu; p_1; \varphi_1)$:

$$A(\mu; p_1; \varphi_1) = A(\mu; p_1; -\varphi_1) = A(\mu; p_1; \pi - \varphi_1)\,,$$
$$\Phi(\mu; p_1; \varphi_1) = \Phi(\mu; p_1; -\varphi_1) = -\Phi(\mu; p_1; \pi - \varphi_1)\,, \tag{24}$$

reduces the range of required azimuthal angles φ_1 to [0, π/2]. Our numerical MSH calculations show that azimuthal dependence of function $\Psi_L(\mu; p_1; \varphi_1)$ is very smooth and relatively weak. This suggests that $\Psi_L(\mu; p_1; \varphi_1)$ can be found for an arbitrary angle φ_1 by linear interpolation over a relatively sparse grid from the range [0, π/2].

The described properties reduce the size of the aerosol LUT of OTF_L to 5 dimensions: {x_1, τ, p_1, μ, φ_1}. We calculated the final aerosol LUT with ω_0=1 and H_0^{eq}=1.5 *km* for the following grids of parameters: 11 values of the asymmetry parameter, x_1={1.2, 1.3, …, 2.2} that cover the typical range of natural variability of aerosol phase function; 18 equidistant values of aerosol optical thickness, τ^a={0.05, 0.1, …, 0.85, 0.9}; 40 values of spatial frequency, p_1={0, …, 150}. Our calculations show that spatial frequencies beyond this range contribute less than ~10^{-3}-10^{-4} of the variation $\tilde{L}_s^d(r; s_0, s)$, and $p_{\text{Nyquist}}=\frac{\pi}{0.03}\cong 105$ is sufficient for calculations with the Landsat spatial resolution of 30 m. The LUT is calculated for 8 view zenith angles, μ={-0.3, -0.4, …, -1} and 10 azimuths $\varphi_1=\frac{\pi}{180}\{0^o, 10^o, \ldots, 90^o\}$. The amplitude and phase of OTF are stored to four significant digits as scaled integers in the binary format. With these arrangements, the size of the LUT is 3.9 Mb.

The LUT navigation algorithm chooses the nearest value of the asymmetry parameter x_1, and uses linear interpolation in τ and μ for all p_1 and φ_1. Then, it rescales spatial frequency to adjust the height of aerosol layer. These steps prepare the aerosol OTF $\Psi_L^a(\mu; p_1; \varphi_1)$ for the specified view zenith angle and aerosol parameters, except single scattering albedo, which is adjusted on the next step.

3.3 Calculation of OTF for the Aerosol-Molecular Mixture

The common practice of radiative transfer is to handle the scattering by different atmospheric components, such as aerosols and air molecules, by linearly mixing their optical properties according to respective fractional contributions, $f^a=\frac{\tau^a}{\tau}$, $f^m=\frac{\tau^m}{\tau}$:

$$\tau=\tau^a+\tau^m,\ \omega=f^a\omega^a+f^m\omega^m,\ \chi(\gamma)=(f^a\omega^a\chi^a(\gamma)+f^m\omega^m\chi^m(\gamma))/\omega. \qquad (25)$$

The radiative transfer problem is then solved with the average properties. As we showed above, for the medium-to-high frequencies *p*, the OTF is accurately represented by its single scattering component. The linear mixing method (LMM) was shown to be exact in such conditions for the TOA path radiance[14],

$$D(\tau)=f^aD^a(\tau)+f^mD^m(\tau), \qquad (26)$$

because $\tau\omega\chi(\gamma)=\tau^a\omega^a\chi^a(\gamma)+\tau^m\omega^m\chi^m(\gamma)$. The key detail of LMM is to mix the path radiance components calculated for the same optical thickness τ. A simple analysis of the single scattering solution for OTF (Eq. 19a) shows that LMM would have worked in our case if the vertical profiles of aerosols and molecules (air density) were the same. It is known, however, that the equivalent heights of the aerosol and molecular atmospheres are very different, 0.5-2 km vs ≈8 km, respectively. In order to use linear mixing, we represent the atmosphere by two layers with aerosols at the bottom. Then, LMM can be applied to the bottom layer,

$$Z(z_1,H)=f^aZ^a(z_1,H)+f^mZ^m(z_1,H). \qquad (27)$$

After that, OTF at TOA is found by adding the molecular contribution of the top layer (Eq. 20).

To implement this approach, we calculated two more LUTs OTF_L for the top and bottom layers of the molecular atmosphere, $Z^m(0,z_1)$ and $Z^m(z_1,H)$, where z_1=1.5 km to agree with the aerosol LUT. Thus, the molecular LUTs have four dimensions, $\{\tau, p_1, \mu, \varphi_1\}$. The implemented τ-grid serves the range of wavelengths from 0.4 μm and higher.

As a summary, the LUT mixing algorithm performs the following operations:

- finds Rayleigh OTF for two layers, $Z^m(z_1,H)$ and $Z^m(0,z_1)$, where z_1 is defined from the height of aerosol layer, H- H_a^{eq} = z_1;
- adjust the single scattering albedo of aerosol ω^a for the bottom layer (Eqs. 22);
- mixes molecular and aerosol contributions for the bottom layers (Eq. 27);
- calculates atmospheric OTF_L at TOA by adding contribution of the top molecular layer (Eq. 20).

Finally, the function $\Psi_L(\mu; p_x, p_y, \varphi)$ is reconstructed from $\Psi_L(\mu; p_1, \varphi_1)$ based on Eqs. (23-24).

4. Discussion

With introduced parameterizations we achieve a very high efficiency of the algorithm when any further improvements can only be of an incremental nature. With the intermediate functions (Eqs. (9-11)) calculated once, computing the second and third terms of Eq. (1) requires only several additive/multiplicative operations per pixel. The variational term of Eq. (1) requires two 2D Fourier transforms: the first (direct) transform calculates spatial spectrum of variation of surface albedo, and the second (inverse) transform restores the spatial variation of the TOA radiance. These operations are efficiently performed with the FFT algorithm[16] that takes $N\log_2 N$ operations for the image with N^2 pixels. The selected Fourier-transform approach based on OTF is more efficient than the approach with spatial integration of the atmospheric PSF that requires ~N^2 operations. In summary, for small images the computing time is entirely defined by the 1D radiative transfer calculations of code SHARM. For the large images, the overall time is affected by calculation of the last variational term of Eq. (1).

In order to realistically model reflectance of inland rivers and lakes, especially in the glint area, we are also using the BRF model of Nakajima and Tanaka. The wind speed is assumed constant across the image. One can also specify the variable Lambertian offset for the water pixels for an approximate modeling reflectance of suspended matter or reflectance from the shallow bottom.

A discussion on the accuracy of 1D code SHARM[15], for example choice of parameter *nb*, applies to code SHARM-3D only in regard to the 1D radiative transfer calculations. The overall accuracy of this code (~1%) is largely defined by the parameterizations used.

Because it neglects the non-linear interactions in variation of surface reflectance, code SHARM-3D should not be used at resolutions or scales of inhomogeneity typical of establishing the 1D radiative transfer regime, e.g. 3-5 km. In these conditions, SHARM-3D produces systematic biases for pixels that are brighter or darker than the average. The magnitude of biases, which tend to reduce the contrast of calculated radiance, may reach several percent. This is easy to demonstrate on an example of Lambertian surface. Over the large homogeneous areas of the image, the multiple reflections from the surface enhance the surface-reflected radiance proportionally to the albedo of this particular area, $(1-q^{area}c_0)^{-1}$. At the same time, our linearized solution (Eq. (1)) calculates this enhancement as proportional to the albedo averaged over the whole image, $(1-\bar{q}c_0)^{-1}$, which leads to the mentioned biases.

To allow the user make calculations in 1D regime, we implemented an independent pixel approximation (IPA) as a separate mode of calculations. The mode is specified in the surface properties file (*.sfc) by parameter szDimRT, which can take a value of either “1D” or “3D”. The algorithm behind IPA is a rigorous 1D Green’s function method[6] which has the same accuracy as code SHARM, but becomes progressively faster with the increase of the image size. The IPA algorithm does not use parameterizations. Instead, it achieves a rigorous convergence for the series of multiple reflections for each surface pixel. For this reason, the “1D” mode is considerably slower than “3D” mode. Table 1 illustrates the relative speed of 3D solution vs IPA (1D) solutions of code SHARM-3D and of 1D code SHARM for the images of different size.

As a brief summary, let us list the main features of code SHARM-3D. This code was developed for fast and accurate simulations of the monochromatic radiance at the top of the atmosphere over spatially variable surfaces with Lambertian or anisotropic reflectance. The code also calculates the distribution of surface albedo corresponding to given SZA, atmospheric conditions, and BRF distribution. The surface boundary condition is periodic. The atmosphere is laterally uniform, and consists of two vertical slabs with aerosols in the bottom layer. Code SHARM-3D performs simultaneous calculations for all specified incidence-view geometries, and multiple wavelengths in one run. The range of view zenith angles is presently limited by the maximal value of μ=-0.3 in look-up table of pre-computed OTF_L ($\theta \le 72.5^o$). Also, the maximal LUT value of total optical thickness of atmosphere is 0.9. If τ>0.9, we assume that $OTF_L(\tau)=OTF_L(0.9)$. This assumption has little impact on the accuracy of radiance calculations because *i*) all other terms are calculated accurately, *ii*) the path radiance dominates the total TOA radiance at high optical thickness, and *iii*) the relative contribution of the variational term $\tilde{L}_s^d(r; s_0, s)$ decreases with τ proportionally to the decrease of the surface irradiance.

The details on the input parameters are provided in the document “SHARM Manual”.

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N	32	64	128	256	512	1024
3D/SHARM	2.8	3.2	4.5	10.0	37.1	143.3
IPA/SHARM	6.2	16.8	59.1	227.6	902.9	3605

Table 1. **Relative efficiency of code SHARM-3D in 3D and IPA modes**.
The second and third rows show the ratio of computing time of code SHARM-3D in 3D and IPA modes to the time of a single-pixel solution of 1D code SHARM, for the images of different size.
The top row gives the linear dimension of an image (the image size is N^2). The calculations were performed for anisotropic surface, medium opacity atmosphere, and off-nadir view geometry (SZA=60^o, μ=-0.7, φ=0). The reference time of a SHARM solution on PC DELL Precision 650 was 0.078 sec.

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